NASTRAN SOLUTIONS OF PROBLEMS DESCRIBED BY SIMULTANEOUS PARABOLIC DIFFERENTIAL EQUATIONS

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INTRODUCTION

NASTRAN solution techniques are shown for a numerical analysis of a class of coupled vector flow processes described by simultaneous parabolic differential equations. To define one physical problem type where equations of this form arise, the differential equations describing the coupled transfers of heat and mass in mechanical equilibrium with negligible mass average velocity are presented and discussed. Also shown are the equations describing seepage when both electrokinetic and hydrodynamic forces occur. Based on a variational statement of the general problem type, the concepts of scalar transfer elements and parallel element systems are introduced. It is shown that adoption of these concepts allows the direct use of NASTRAN's existing Laplace type elements for uncoupled flow (i.e., the heat transfer elements) for treating multi-component coupled transfer. Sample problems are included which demonstrate the application of these techniques for both steady-state and transient problems.

IRREVERSIBLE THERMODYNAMICS

Based on the linear phenomenological laws of irreversible thermodynamics and the general conservation laws, generalized flow equations describing the simultaneous transfer of vector processes may be developed. A brief development for coupled energy and mass flow is presented here and the reader is referred to the literature [references 1 to 8] for more details and applications.

Consider a motionless fluid, i.e., a fluid with zero or negligible mass average velocity, consisting of N chemical components K and contained in a mathematically well-defined geometric volume V which is separated from its surroundings by an equally well-defined boundary surface S. Within this system the coupled diffusion of matter and energy takes place. Assume that no chemical reactions are occurring and that the effects of external forces and viscous phenomena may be neglected. For this nondeforming system, therefore, the diffusion of momentum and its associated conservation law need not be directly considered. The conservation laws of mass and energy are applicable.

Adopting the repeated indices summation convention on i, j and designating rectangular Cartesian coordinates as x_i, the conservation of energy for the system under consideration can be written as

$$\rho C \frac{\partial T}{\partial t} = -\frac{\partial J_i^q}{\partial x_i} \tag{1}$$

and the conservation of mass as

$$\rho \frac{\partial C_K}{\partial t} = -\frac{\partial J_i^K}{\partial x_i} \quad (K = 1,2,\ldots,N) \tag{2}$$

where

C = specific heat
C_K = mass fraction of chemical component K ($C_K = \frac{\rho_K}{\rho}$)
J_i^q = i^{th} spacial component of the heat flux vector with respect to the mass average velocity
J_i^K = i^{th} spacial component of the diffusion flux vector of chemical component K with respect to the mass average velocity
t = time
T = absolute temperature
ρ = total mass density
ρ_K = mass density of chemical component K

The conservation equations (1) and (2) are of similar form and can be generalized to account for distributed external sources. Thus, a general conservation law for the M generalized fluxes γ can be written as

$$\rho C_\gamma \frac{\partial f_\gamma}{\partial t} = -\frac{\partial J_i^\gamma}{\partial x_i} + Q_\gamma \quad (\gamma = 1,2,\ldots,M) \tag{3}$$

where

C_γ = specific mass capacity for flux γ
J_i^γ = i^{th} spacial component of the γ^{th} generalized flux vector with respect to the mass average velocity
f_γ = scalar thermodynamic potential corresponding to flux γ
Q_γ = external source strength corresponding to flux γ

According to the linear laws of irreversible thermodynamics, the M generalized fluxes $\vec{J}^{\gamma}$ result from the action of M generalized forces $\underline{\vec{X}}_{\varepsilon}$ ($\varepsilon = 1, 2, \ldots M$) and are proportional to these forces. For general anisotropic coupled transfer, therefore, we may write

$$J_i^{\gamma} = -\sum_{\varepsilon=1}^{M} L_{\gamma i}^{\varepsilon j} \underline{\bar{X}}_{\varepsilon j} \tag{4}$$

where

$\underline{\bar{X}}_{\varepsilon j}$ = j^{th} spacial component of the ε^{th} generalized thermodynamic force

$L_{\gamma i}^{\varepsilon j}$ = phenomenological coefficient expressing the effects of the j^{th} component of the thermodynamic force $\underline{\vec{X}}_{\varepsilon}$ on the i^{th} component of the flux $\vec{J}^{\gamma}$

In addition, it can be shown that the appropriate selection of fluxes and forces through examination of the local rate of entropy production leads to the important results:

$$L_{\gamma i}^{\varepsilon j} = L_{\varepsilon j}^{\gamma i} \tag{5}$$

$$\underline{\bar{X}}_{\varepsilon j} = \eta_{\varepsilon} \frac{\partial f_{\varepsilon}}{\partial x_j} \tag{6}$$

where

η_{ε} = proportionality factor depending on the choice of generalized thermodynamic fluxes and forces; η_{ε} is assumed constant for the range of operating conditions considered here.

That is, the phenomenological coefficient matrix is symmetric and the generalized thermodynamic forces are expressible as gradients of the scalar potentials. When written in the above form, the quantities are known as Onsager coefficients.

Combining equations (3), (4) and (6) results in a general set of simultaneous differential equations of the parabolic type describing the coupled irreversible transfer phenomena

$$\rho C_\gamma \frac{\partial f_\gamma}{\partial t} = \frac{\partial}{\partial x_i}\left[\sum_{\varepsilon=1}^{M} L_{\gamma i}^{\varepsilon j}\, \eta_\varepsilon \frac{\partial f_\varepsilon}{\partial x_j}\right] + Q_\gamma \qquad (\gamma = 1,2,\ldots,M) \tag{7}$$

For the case of isotropic transfer equations (4) and (7) become, respectively

$$J_i^\gamma = -\sum_{\varepsilon=1}^{M} L_\gamma^\varepsilon \overline{\overline{X}}_{\varepsilon i} \tag{8}$$

$$\rho C_\gamma \frac{\partial f_\gamma}{\partial t} = \frac{\partial}{\partial x_i}\left[\sum_{\varepsilon=1}^{M} L_\gamma^\varepsilon\, \eta_\varepsilon \frac{\partial f_\varepsilon}{\partial x_i}\right] + Q_\gamma \qquad (\gamma = 1,2,\ldots M) \tag{9}$$

Equations (9) in their most simple form may be used to describe the steady-state diffusion of uncoupled heat or mass in an isotropic medium. In their most general form, equations (7) may be utilized to describe the transient diffusion of general anisotropic coupled flows such as multi-component mass and/or heat.

As examples of the above developments, consider first the one-dimensional (i = j = 1) coupled transfer of heat and mass. For this case,

$$\begin{aligned} J_1^1 &= -L_{11}^{11}\overline{\overline{X}}_{11} - L_{11}^{21}\overline{\overline{X}}_{21} \\ J_1^2 &= -L_{21}^{11}\overline{\overline{X}}_{11} - L_{21}^{21}\overline{\overline{X}}_{21} \end{aligned} \tag{10a}$$

where J_1^1 is the heat flux and J_1^2 the mass flux. The coupling term L_{11}^{21} expresses the effects of the concentration gradient on the heat flux while L_{21}^{11} establishes the effects of the temperature gradient on the mass flux. The Onsager coefficient L_{11}^{21} is proportional to the Soret coefficient and L_{21}^{11} to the Dufour coefficient. Recall that $L_{11}^{21} = L_{21}^{11}$.

The equations describing coupled electrokinetic and hydrodynamic flow in porous media offer a second example. In reference 9 a finite element approach is used to analyze the movement of fluid relative to a solid phase and the migration of ionized soil particles relative to a fluid phase, both occurring in an electric force field. For this case,

$$J_i^1 = -\sum_{\varepsilon=1}^{2} L_1^{\varepsilon} \bar{\underline{X}}_{\varepsilon i}$$

$$J_i^2 = -\sum_{\varepsilon=1}^{2} L_2^{\varepsilon} \bar{\underline{X}}_{\varepsilon i} \qquad (10b)$$

where J_i^1 is the i^{th} component fluid discharge velocity and J_i^2 is the i^{th} component of the current density. The coefficient L_1^1 expresses the effects of hydrostatic potential gradients $\bar{\underline{X}}_{1i}$ on the discharge velocities while L_2^2 expresses the effects of voltage gradient $\bar{\underline{X}}_{2i}$ on the current. The L_1^2 and L_2^1 terms express the cross coupling between voltage gradient and fluid velocity and between potential gradient and electrical current, respectively.

VARIATIONAL FORMULATION

Equation (7) is a set of simultaneous parabolic differential equations describing the coupled transport processes in the continuum. While a Galerkin approach can be employed in a straightforward manner to evolve a finite element statement of the problem, the approach used here is based on a variational formulation similar to the principle of virtual work used in mechanics. Because of this similarity, it is designated as a principle of virtual generalized work and has the advantage that physical interpretation can be associated with its use.

Consider the motionless fluid within the well-defined boundary. For each flow quantity γ, the boundary of the volume V in which the M generalized fluxes are transferred may be considered as consisting of three regions S_1, S_2 and S_3 as follows:

1. Over the boundary S_1 the flux $\tilde{J}_i^{\gamma}$ is prescribed.
2. Over the boundary S_2 the generalized convective flux $\approx{J}_i^{\gamma}$ is proportional to the thermodynamic potential differences between the boundary values $(\eta_\gamma f_\gamma)_{S_2}$ and the <u>known</u> ambient values $(\eta_\gamma f_\gamma)_\infty$.

3. Over the boundary S_3 the thermodynamic potential $(\eta_\gamma f_\gamma)_{S_3}$ is prescribed.

Now allow a fictitious variational change $\eta_\gamma \delta f_\gamma$ which does not violate the constraints of the system; i.e., $\eta_\gamma \delta f_\gamma$ is zero over S_3 and arbitrary elsewhere. Also, the virtual changes are assumed to occur without the passage of time while the various fluxes remain constant.

For this volume consider the sum of the products of the generalized fluxes J_i^γ and the variations in their conjugate thermodynamic potentials $\eta_\gamma \delta f_\gamma$, that is, the virtual generalized work

$$\sum_{\gamma=1}^{M} J_i^\gamma \, (\eta_\gamma \delta f_\gamma) \tag{11}$$

Integration of equation (11) over the total boundary area S and application of Gauss' Theorem yields

$$\int_S \sum_{\gamma=1}^{M} (J_i^\gamma \eta_\gamma \delta f_\gamma) \nu_i \, dS = \int_V \sum_{\gamma=1}^{M} \frac{\partial J_i^\gamma}{\partial x_i} (\eta_\gamma \delta f_\gamma) dV + \int_V \sum_{\gamma=1}^{M} J_i^\gamma \frac{\partial (\eta_\gamma \delta f_\gamma)}{\delta x_i} \, dV \tag{12}$$

where ν_i = i^{th} component of the unit vector along the outer normal to S. Since the general conservation of the various transfer quantities must apply, equation (7) is substituted for the first integral on the right-hand side of equation (12), yielding

$$\int_V \sum_{\gamma=1}^{M} J_i^\gamma \, \eta_\gamma \frac{\partial (\delta f_\gamma)}{\partial x_i} \, dV + \int_V \sum_{\gamma=1}^{M} \left(Q_\gamma - \rho C_\gamma \frac{\partial f_\gamma}{\partial t} \right) \eta_\gamma \delta f_\gamma dV$$

$$+ \int_{S_1} \sum_{\gamma=1}^{M} \bar{J}^\gamma \, (\eta_\gamma \delta f_\gamma) dS + \int_{S_2} \sum_{\gamma=1}^{M} \bar{\bar{J}}^\gamma \, (\eta_\gamma \delta f_\gamma) dS = 0 \tag{13}$$

Note that the surface integral appearing in equation (13) extends only over that portion of the boundary for which δf_γ is not prescribed and that the scalar

boundary fluxes per unit surface area

$$\begin{aligned} \overline{J}^{\gamma} &= -\tilde{J}_i^{\gamma}\nu_i \\ \overline{\overline{J}}^{\gamma} &= -\tilde{\tilde{J}}_i^{\gamma}\nu_i \end{aligned} \tag{14}$$

have been employed in writing this equation. In addition, it should be noted that the generalized convective flux can be expressed in terms of the thermodynamic potential differences in the form

$$\overline{\overline{J}}^{\gamma} = \sum_{\varepsilon=1}^{M} h_{\varepsilon}^{\gamma} \left[(\eta_{\varepsilon} f_{\varepsilon})_{\infty} - (\eta_{\varepsilon} f_{\varepsilon})_{S_2}\right] \tag{15}$$

where

h_{ε}^{γ} = proportionality factor expressing the contribution from the ε^{th} thermodynamic potential difference to the flux $\overline{\overline{J}}^{\gamma}$ at the boundary S_2

The characteristics of the variational statement (13) are such that its Euler equations and boundary conditions are those governing the case of coupled vector transfer considered here when the expressions (4) or (8) are employed. As such, it may be viewed as an alternate expression of the mathematical problem posed by equations (7) or (9) and the associated boundary conditions discussed above. These results indicate the similarities between the variational principle for the coupled irreversible processes and the principle of virtual work for mechanical systems. From this presentation the analogies between the variation in thermodynamic potentials (or state variables) and mechanical deformations, between surface flux and mechanical surface forces, and between thermodynamic sources/sinks and mechanical body forces are clearly indicated.

GENERAL FINITE ELEMENT FORMULATION

For irreversible coupled flows, the thermodynamic potentials at the grid points of the element are taken as the degrees of freedom. Element properties are determined using the principle of virtual generalized work together with functions expressing the state of the thermodynamic potentials within the element in terms of their grid point values. With this information the gradients of the potentials and alternately the various fluxes within the element may be uniquely defined in terms of the grid point values of the potentials. Assembly of the element equations to describe the complete system is accomplished with

the aid of the variational principle. This assembly is accomplished by requiring that the thermodynamic potentials be compatible between elements and that flow conservation apply at the grid points. In essence, only compatible states are considered and the true values of the potential are those for which flow conservation holds, a condition which is enforced by the principle of virtual generalized work.

Details of the general finite element formulation are presented in reference 8 and only the form of the resulting matrix equations of motion describing the coupled processes are presented here as follows:

$$[D]\{\frac{dP_\alpha}{dt}\} + ([K] + [K_C])\{P_\alpha\} = \{F_Q\} + \{F_B\} + \{F_C\} \tag{16}$$

where

$\{P_\alpha\}$ = values of the thermodynamic potentials at the α grid points of the assembled model
$[D]$ = generalized capacitance matrix for the assembled model
$[K]$ = generalized conduction matrix for the assembled model
$[K_C]$ = generalized boundary convection matrix for the assembled model
$\{F_Q\}$ = generalized source vector for the assembled model
$\{F_B\}$ = generalized boundary flux vector for the assembled model
$\{F_C\}$ = generalized boundary convection vector for the assembled model

Note that $\{P_\alpha\}$ is a column vector of length equal to the number of grid points of the assembled model times the number of transport quantities (i.e., $\alpha \times M$).

NASTRAN SOLUTIONS

The previous developments are general in nature and can be applied for the finite element description of coupled anisotropic transfer in one, two and three dimensions. Once suitable interpolation functions have been chosen, the finite element matrices can be obtained and assembled to form the set of equations (16) describing the idealized system using well-known procedures (refs. 8 and 9). In what follows, the reader will be assumed familiar with these procedures and the discussion will center on special techniques which may be employed to permit the direct use of NASTRAN for the analysis of M coupled transfer processes.

One-Dimensional Element Formulation

A one-dimensional element suitable for use in the analysis of two coupled flows is presented below and shown to be equivalent to a combined system

of parallel one-dimensional Laplace elements, representing uncoupled transfer, connected by "scalar transfer elements," representing coupling. With this information the extension to the case of M coupled flows is discussed.

Consider a one-dimensional finite element of constant cross-sectional area A connecting grid points ξ and θ on the x axis. Assume a linear variation in the two thermodynamic potential variables $p_1(x,t)$ and $p_2(x,t)$ along the axis of the element. Thus,

$$\begin{aligned} p_1 &= \eta_1 f_1 = \bar{a} + \bar{b}x \\ p_2 &= \eta_2 f_2 = \bar{c} + \bar{d}x \end{aligned} \tag{17}$$

where $\bar{a}(t)$, $\bar{b}(t)$, $\bar{c}(t)$ and $\bar{d}(t)$ are generalized coordinates which can be related to the four unknown grid point values of the thermodynamic potentials, i.e., p_1^{ξ}, p_1^{θ}, p_2^{ξ}, p_2^{θ}, using equation (17). Evaluating the generalized coordinates in terms of the grid point potential values results in the matrix equation

$$\begin{Bmatrix} p_1 \\ p_2 \end{Bmatrix} = \left[\begin{array}{c|c|c|c} 1 + \frac{x_\xi}{\ell} - \frac{x}{\ell} & \frac{x}{\ell} - \frac{x_\xi}{\ell} & 0 & 0 \\ \hline 0 & 0 & 1 + \frac{x_\xi}{\ell} - \frac{x}{\ell} & \frac{x}{\ell} - \frac{x_\xi}{\ell} \end{array}\right] \begin{Bmatrix} p_1^{\xi} \\ p_1^{\theta} \\ p_2^{\xi} \\ p_2^{\theta} \end{Bmatrix} \tag{18}$$

where

p_1^{ξ} = value of the thermodynamic potential p_1 at grid point ξ, etc.

ℓ = length of element ($\ell = x_\theta - x_\xi$)

x_ξ, x_θ = coordinates of element end points

For two coupled flows, the Onsager coefficient matrix can be written as

$$\left[\begin{array}{c|c} L_{11} & L_{12} \\ \hline L_{12} & L_{22} \end{array}\right] \tag{19}$$

Using equations (18) and (19), a generalized conduction matrix for the element is found in reference 8 as

$$[K^e] = \frac{A}{\ell} \begin{bmatrix} L_{11} & -L_{11} & L_{12} & -L_{12} \\ -L_{11} & L_{11} & -L_{12} & L_{12} \\ L_{12} & -L_{12} & L_{22} & -L_{22} \\ -L_{12} & L_{12} & -L_{22} & L_{22} \end{bmatrix} \tag{20}$$

The one-dimensional element for the analysis of two coupled processes has two grid points and two degrees of freedom at each of these points. This representation results in the four by four element matrix (20) which may be partitioned into the form

$$[K^e] = \frac{A}{\ell} \left[\begin{array}{c|c} K^e_{11} & K^e_{12} \\ \hline K^e_{12} & K^e_{22} \end{array}\right] \tag{21}$$

with

$$[K^e_{11}] = \left[\begin{array}{c|c} L_{11} & -L_{11} \\ \hline -L_{11} & L_{11} \end{array}\right] \tag{22}$$

$$[K^e_{22}] = \left[\begin{array}{c|c} L_{22} & -L_{22} \\ \hline -L_{22} & L_{22} \end{array}\right] \tag{23}$$

$$[K^e_{12}] = \left[\begin{array}{c|c} L_{12} & -L_{12} \\ \hline -L_{12} & L_{12} \end{array}\right] \tag{24}$$

Examination of these indicates that $[K^e_{11}]$ represents the two by two element matrix describing the uncoupled transfer of J^1 through the thermodynamic potential gradient in $p_1 = \eta_1 f_1$. Similarly, $[K^e_{22}]$ is the two by two matrix describing the uncoupled transfer of J^2 through the gradient in $p_2 = \eta_1 f_1$. While $[K^e_{12}]$ is the two by two matrix representing coupling between the two processes. At this point, it is useful to introduce the concept of a "scalar transfer element" which may connect any two degrees of freedom and is defined by the two by two generalized conductivity matrix

$$[K_s] = \begin{matrix}\text{Scalar transfer element} \\ \text{conductivity matrix}\end{matrix} = k \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{25}$$

where

k = conductivity of the scalar transfer element

With the above observations and use of the scalar transfer element concept, it can be shown that a "parallel element system" composed of two one-dimensional Laplace elements (i.e., NASTRAN ROD heat transfer elements) connected by four scalar transfer elements (i.e., SCALAR CONDUCTION elements), see Figure 1, can be utilized to represent the single coupled transfer element of equation (20).

This new model has four grid points with one degree of freedom at each point. Grid points ξ and θ are connected by ROD 1 of area A and length $\ell = x_\theta - x_\xi$. The degree of freedom at grid point ξ is p_1^ξ and at grid point θ is p_1^θ. The element properties of ROD 1 are those of equation (22) and represent the uncoupled transfer of $\vec{J}^1$. ROD 2 is also of length ℓ and area A (since the geometric location of ξ' is identical to ξ and θ' identical to θ) and represents the uncoupled transfer of $\vec{J}^2$ between p_2^ξ and p_2^θ at grid points ξ' and θ' as given by equation (23). The four scalar transfer elements represent the effects of coupling as described by equation (24). The conductivities of these are

$$\begin{aligned} k_1 &= \begin{matrix}\text{Generalized conductivity of} \\ \text{SCALAR 1 transfer element}\end{matrix} = -\frac{A}{\ell} L_{12} \\ k_2 &= \begin{matrix}\text{Generalized conductivity of} \\ \text{SCALAR 2 transfer element}\end{matrix} = \frac{A}{\ell} L_{12} \end{aligned} \tag{26}$$

Several advantages are gained using this assembly. One advantage is that physical insight is gained into this complex transfer problem. Another is that existing Laplace finite elements, like those in NASTRAN for the analysis of uncoupled heat transfer processes, can be utilized for the parallel models of the primary flows and then interconnected by the scalar transfer elements. A

third advantage to be gained is that a simple and practical method to automate in the computer for treating an arbitrary number of M coupled processes is to model the primary uncoupled flows by M parallel systems using existing NASTRAN elements and to then automatically interconnect these with scalar transfer elements representing the coupling.

Two-Dimensional Element Formulation

The developments will now be extended to the case of coupled two-dimensional isotropic flow. The most general element for use in the investigation of two-dimensional flow is a triangle of thickness $\bar{t}$. Two coupled flows will be considered for a triangular element lying in the xy plane and defined by the three grid points (ξ, θ, ϕ) with six unknown degrees of freedom.

Proceeding as before, assume that the potentials $p_1(x,y,t)$ and $p_2(x,y,t)$ are distributed linearly within the element by the relations

$$\begin{aligned} p_1 &= \bar{a} + \bar{b}x + \bar{c}y \\ p_2 &= \bar{d} + \bar{e}x + \bar{f}y \end{aligned} \tag{28}$$

where $\bar{a}(t)$, $\bar{b}(t)$, . . . , $\bar{f}(t)$ are again generalized coordinates. Anticipating the results from the one-dimensional parallel element system, it is chosen here to express the Onsager coefficient matrix for two coupled isotropic flows as the sum of three matrices

$$[L^e] = [L_1^e] + [L_2^e] + [L_3^e] \tag{29}$$

where

$$[L_1^e] = \begin{bmatrix} L_{11} & 0 & 0 & 0 \\ 0 & L_{11} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{30}$$

$$[L_2^e] = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & L_{22} & 0 \\ 0 & 0 & 0 & L_{22} \end{bmatrix} \tag{31}$$

$$[L_3^e] = \begin{bmatrix} 0 & 0 & L_{13} & 0 \\ 0 & 0 & 0 & L_{13} \\ L_{13} & 0 & 0 & 0 \\ 0 & L_{13} & 0 & 0 \end{bmatrix} \tag{32}$$

From the previous results and the form of equations (30) and (31), it is concluded that the uncoupled transfer of $\vec{J}^{\,1}$ and $\vec{J}^{\,2}$ may be included by two parallel Laplace triangular elements of a type available in NASTRAN. With this approach, only the $[L_3^e]$ contribution of equation (32) due to coupling need be presented here.

Using equations (28) and (32) and employing standard procedures lead to the element matrix $[K]_{coupling}$ representing between the parallel element system (see reference 8), thus

$$[K]_{coupling} = \frac{\bar{t}L_{13}}{4\Delta} \begin{bmatrix} 0 & 0 & 0 & K_{\xi\xi'} & K_{\xi\theta'} & K_{\xi\phi'} \\ 0 & 0 & 0 & K_{\xi\theta'} & K_{\theta\theta'} & K_{\theta\phi'} \\ 0 & 0 & 0 & K_{\xi\theta'} & K_{\theta\phi'} & K_{\phi\phi'} \\ K_{\xi\xi'} & K_{\xi\theta'} & K_{\xi\theta'} & 0 & 0 & 0 \\ K_{\xi\theta'} & K_{\theta\theta'} & K_{\theta\phi'} & 0 & 0 & 0 \\ K_{\xi\phi'} & K_{\theta\phi'} & K_{\phi\phi'} & 0 & 0 & 0 \end{bmatrix} \tag{33}$$

where

$$K_{\xi\xi'} = b_\xi^2 + c_\xi^2 \quad ; K_{\theta\theta'} = b_\theta^2 + c_\theta^2$$

$$K_{\xi\theta'} = b_\xi b_\theta + c_\xi c_\theta ; K_{\theta\phi'} = b_\theta b_\phi + c_\theta c_\phi$$

$$K_{\xi\phi'} = b_\xi b_\phi + c_\xi c_\phi ; K_{\phi\phi'} = b_\phi^2 + c_\phi^2$$

and

$$a_\xi = x_\phi y_\theta - x_\theta y_\phi$$

$$b_\xi = y_\phi - y_\theta$$

$$c_\xi = x_\theta - x_\phi$$

(etc., in cyclic order ξ, θ, ϕ)

Δ = area of the triangular element

x_ξ, y_ξ = coordinates of element corner points, etc.

With the above results a parallel element system composed of two NASTRAN heat transfer triangular elements and connected by scalar transfer elements can be constructed, see Figure 2. Grid points ξ, θ, ϕ are connected by TRIANGLE 1 of thickness $\bar{t}$ and properties $[L_1^e]$ of equation (30). Grid points ξ', θ', ϕ' are connected by TRIANGLE 2 also of thickness $\bar{t}$ but with properties $[L_2^e]$ of equation (31). The two triangular elements are connected by nine scalar transfer elements with properties $[K]_{coupling}$* obtained from equation (33). The extension to three-dimensional problems is not difficult since one need only utilize existing three-dimensional heat transfer elements in the program for the uncoupled parallel flows and utilize the variational principle and the scalar transfer elements to include the effects of thermodynamic coupling.

SAMPLE PROBLEMS

Two sample problems are presented to demonstrate aspects of the above developments. Parallel and scalar transfer elements are employed and solutions obtained using the NASTRAN program.

Problem 1 - One-Dimensional Steady-State Process, Three Coupled Flows

The one-dimensional transfer of $\vec{J}^{\,1}$, $\vec{J}^{\,2}$, and $\vec{J}^{\,3}$ along the x axis of a continuum due to gradients in the potentials $p_1(x)$, $p_2(x)$, and $p_3(x)$ is considered. Find the steady-state distributions in the potentials. The continuum is of length L = 4.0 and cross-sectional area A = 1.0, and there is internal generation within the continuum given by

*$K_{\xi\xi'}$ is the generalized conductivity for the scalar transfer element connecting degree of freedom ξ with degree of freedom ξ', etc.

$$Q_1(x) = -(4.6 + 1.2x)$$
$$Q_2(x) = 24.4 - 1.8x \qquad (34)$$
$$Q_3(x) = 1.0 - 12.0x$$

The boundary conditions are specified as

$$\begin{aligned} p_1(0) &= 0.0 & p_1(4) &= 32.0 \\ p_2(0) &= 0.0 & p_2(4) &= -48.0 \\ p_3(0) &= 0.0 & p_3(4) &= 64.0 \end{aligned} \qquad (35)$$

and the Onsager relations have been determined as

$$\begin{Bmatrix} J_x^1 \\ J_x^2 \\ J_x^3 \end{Bmatrix} = - \begin{bmatrix} 1.0 & -0.1 & 0.2 \\ -0.1 & 4.0 & 0.3 \\ 0.2 & 0.3 & 2.0 \end{bmatrix} \begin{Bmatrix} \partial p_1/\partial x \\ \partial p_2/\partial x \\ \partial p_3/\partial x \end{Bmatrix} \qquad (36)$$

From equations (9), (34), and (36) the equations describing the process are found as

$$1.0 \frac{\partial^2 p_1}{\partial x^2} - 0.1 \frac{\partial^2 p_2}{\partial x^2} + 0.2 \frac{\partial^2 p_3}{\partial x^2} + [-4.6 - 1.2x] = 0$$

$$-0.1 \frac{\partial^2 p_1}{\partial x^2} + 4.0 \frac{\partial^2 p_2}{\partial x^2} + 0.3 \frac{\partial^2 p_3}{\partial x^2} + [24.4 - 1.8x] = 0 \qquad (37)$$

$$0.2 \frac{\partial^2 p_1}{\partial x^2} + 0.3 \frac{\partial^2 p_2}{\partial x^2} + 2.0 \frac{\partial^2 p_3}{\partial x^2} + [1.0 - 12.0x] = 0$$

The solution satisfying equations (37) and the boundary conditions is given by

$$p_1(x) = 2.0x^2 \; ; \; p_2(x) = -3.0x^2 \; ; \; p_3(x) = 1.0x^3 \qquad (38)$$

The finite element model is shown in Figure 3. Figure 3(a) shows the fifteen grid points connected by a total of twelve rod elements of length $\ell = 1.0$, i.e.,

three parallel systems each consisting of four unit-length rod elements and representing, respectively, the three primary flows $\vec{J}^1$, $\vec{J}^2$, and $\vec{J}^3$. Figure 3(b) shows a typical parallel system connecting grid points 2, 2', and 2" (i.e., location x = 1.0) and 3, 3', 3" (i.e., location x = 2.0). The properties of the rod and scalar transfer elements for this system are found using our previous conclusions and are presented in Table 1.

The vector $\{F_Q\}$ representing the effects of distributed sources $Q_1(x)$, $Q_2(x)$, $Q_3(x)$ is obtained by simple lumping procedures and applied to the grid points as thermal loads. The boundary conditions (35) are satisfied by constraining the boundary point potentials to their appropriate values using single point constraints (SPC).

Table 2 presents a comparison between analytical results (AN.) from equation (38) and results from the finite element solution (F.E.).

Problem 2 - Two-Dimensional Transient Process, Two Coupled Flows

The two-dimensional coupled transport of the fluxes $\vec{J}^1$ and $\vec{J}^2$ in a square continuum of planform dimension 4.0 and thickness $\bar{t}$ = 2.0 due to gradients in the potentials $p_1(x,y,t)$, $p_2(x,y,t)$ is considered. Find the transient distribution of the two potentials when there is internal generation within the continuum given by

$$\begin{aligned} Q_1(x,y,t) &= [\sin \tfrac{\pi x}{4} \sin \tfrac{\pi y}{4}][t + t^2] \\ Q_2(x,y,t) &= -[\sin \tfrac{\pi x}{4} \sin \tfrac{\pi y}{4}][t + 3t^2] \end{aligned} \tag{39}$$

The initial and boundary conditions are specified as

$$\begin{aligned} p_1(0,y,t) &= 0.0 \qquad p_2(0,y,t) = 0.0 \\ p_1(4,y,t) &= 0.0 \qquad p_2(4,y,t) = 0.0 \\ p_1(x,0,t) &= 0.0 \qquad p_2(x,0,t) = 0.0 \\ p_1(x,4,t) &= 0.0 \qquad p_2(x,4,t) = 0.0 \end{aligned} \tag{40}$$

The Onsager relations for the isotropic material have been determined as

$$\begin{Bmatrix} J_x^1 \\ J_y^1 \\ J_x^2 \\ J_y^2 \end{Bmatrix} = - \begin{bmatrix} 2.0 & 0.0 & 1.0 & 0.0 \\ 0.0 & 2.0 & 0.0 & 1.0 \\ 1.0 & 0.0 & 4.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 4.0 \end{bmatrix} \begin{Bmatrix} \partial p_1/\partial x \\ \partial p_1/\partial y \\ \partial p_2/\partial x \\ \partial p_2/\partial y \end{Bmatrix} \tag{41}$$

ıd the specific mass capacities as

$$\begin{aligned} \rho C_1 &= 0.61685 \\ \rho C_2 &= 0.61685 \end{aligned} \tag{42}$$

From equations (9), (39), (41), and (42), the equations describing the rocess are found as

$$\begin{aligned} 0.61685 \frac{\partial p_1}{\partial t} &= 2.0 \left[\frac{\partial^2 p_1}{\partial x^2} + \frac{\partial^2 p_1}{\partial y^2}\right] + 1.0 \left[\frac{\partial^2 p_2}{\partial x^2} + \frac{\partial^2 p_2}{\partial y^2}\right] + \left[\sin \frac{\pi x}{4} \sin \frac{\pi y}{4}\right]\left[t+t^2\right] \\ 0.61685 \frac{\partial p_2}{\partial t} &= 1.0 \left[\frac{\partial^2 p_1}{\partial x^2} + \frac{\partial^2 p_1}{\partial y^2}\right] + 4.0 \left[\frac{\partial^2 p_2}{\partial x^2} + \frac{\partial^2 p_2}{\partial y^2}\right] - \left[\sin \frac{\pi x}{4} \sin \frac{\pi y}{4}\right]\left[t + 3t^2\right] \end{aligned} \tag{43}$$

he solution satisfying (43) and the boundary and initial conditions is

$$\begin{aligned} p_1(x,y,t) &= \frac{8.0}{\pi^2} \left[\sin \frac{\pi x}{4} \sin \frac{\pi y}{4}\right] t^2 \\ p_2(x,y,t) &= -\frac{8.0}{\pi^2} \left[\sin \frac{\pi x}{4} \sin \frac{\pi y}{4}\right] t^2 \end{aligned} \tag{44}$$

The finite element model is shown in Figure 4. It consists of two parallel ive by five grid point arrays connected by a total of sixty-four right triangular lements, i.e., thirty-two in each array. The two parallel systems represent, respectively, the two primary flows $\vec{J}^1$ and $\vec{J}^2$. Figure 4(b) shows a typical arallel system connecting grid points 7, 8, and 13 with 7', 8', and 13'. The roperties of the triangular elements and scalar transfer elements for this system

are found using our previous conclusions for triangular and scalar elements. For the 7,8,13 system we find, using equation (33) for the scalar elements, that

$$K_{7,7'} = (b_7^2 + c_7^2)\frac{\bar{t}L_{13}}{4\Delta} = \frac{\bar{t}L_{13}}{4\Delta} \qquad K_{7,8'} = (b_7b_8 + c_7c_8)\frac{\bar{t}L_{13}}{4\Delta} = -\frac{\bar{t}L_{13}}{4\Delta}$$

$$K_{7,13'} = (b_7b_{13} + c_7c_{13})\frac{\bar{t}L_{13}}{4\Delta} = 0 \qquad K_{8,8'} = (b_8^2 + c_8^2)\frac{\bar{t}L_{13}}{4\Delta} = \frac{\bar{t}L_{13}}{2\Delta} \qquad (45$$

$$K_{8,13'} = (b_8b_{13} + c_8c_{13})\frac{\bar{t}L_{13}}{4\Delta} = -\frac{\bar{t}L_{13}}{4\Delta} \qquad K_{13,13'} = (b_{13}^2 + c_{13}^2)\frac{\bar{t}L_{13}}{4\Delta} = \frac{\bar{t}L_{13}}{4\Delta}$$

This information is presented in Table 3.

The vector $\{F_Q\}$ representing the effects of the distributed sources $Q_1(x,y,t)$ and $Q_2(x,y,t)$ was obtained by simple lumping procedures. The boundary and initial conditions (40) were satisfied by constraining the boundary grid point potentials to their appropriate values.

Table 4 presents a representative comparison between analytical results (AN.) from (44) and results from the NASTRAN analysis (F.E.). Numerical integration was performed using 100 time steps with integration interval $t = 0.05$ and maximum error was less than five percent.

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Table 1

Element Connection Table for Parallel System Between Grid Points 2,2',2" and 3,3',3"

Element Type	Connecting Grid Points	A	ℓ	$L_{\gamma\varepsilon}$	$k = I \frac{A}{\ell} L_{\gamma\varepsilon}$
ROD 1	2 - 3	1.0	1.0	$L_{11} = 1.0$	
ROD 2	2'- 3'	1.0	1.0	$L_{22} = 4.0$	
ROD 3	2"- 3"	1.0	1.0	$L_{33} = 2.0$	
Scalar 1	2 - 2'	1.0	1.0	$L_{12} = -0.1$	0.1
Scalar 1	2 - 2"	1.0	1.0	$L_{13} = 0.2$	-0.2
Scalar 1	2'- 2"	1.0	1.0	$L_{23} = 0.3$	-0.3
Scalar 1	3 - 3'	1.0	1.0	$L_{12} = -0.1$	0.1
Scalar 1	3 - 3"	1.0	1.0	$L_{13} = 0.2$	-0.2
Scalar 1	3'- 3"	1.0	1.0	$L_{23} = 0.3$	-0.3
Scalar 2	2 - 3'	1.0	1.0	$L_{12} = -0.1$	-0.1
Scalar 2	2'- 3	1.0	1.0	$L_{12} = -0.1$	-0.1
Scalar 2	2 - 3"	1.0	1.0	$L_{13} = 0.2$	0.2
Scalar 2	2"- 3	1.0	1.0	$L_{13} = 0.2$	0.2
Scalar 2	2'- 3"	1.0	1.0	$L_{23} = 0.3$	0.3
Scalar 2	2"- 3'	1.0	1.0	$L_{23} = 0.3$	0.3

Table 2

Problem 1 Results

Location	$P_1(x)$		$P_2(x)$		$P_3(x)$	
x =	AN.	F.E.	AN.	F.E.	AN.	F.E.
0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.0	2.0	2.0^-	-3.0	-3.0	1.0	1.0^+
2.0	8.0	8.0^-	-12.0	-12.0	8.0	8.0^+
3.0	18.0	18.0^-	-27.0	-27.0	27.0	27.0^+
4.0	32.0	32.0	-48.0	-48.0	64.0	64.0

Table 3

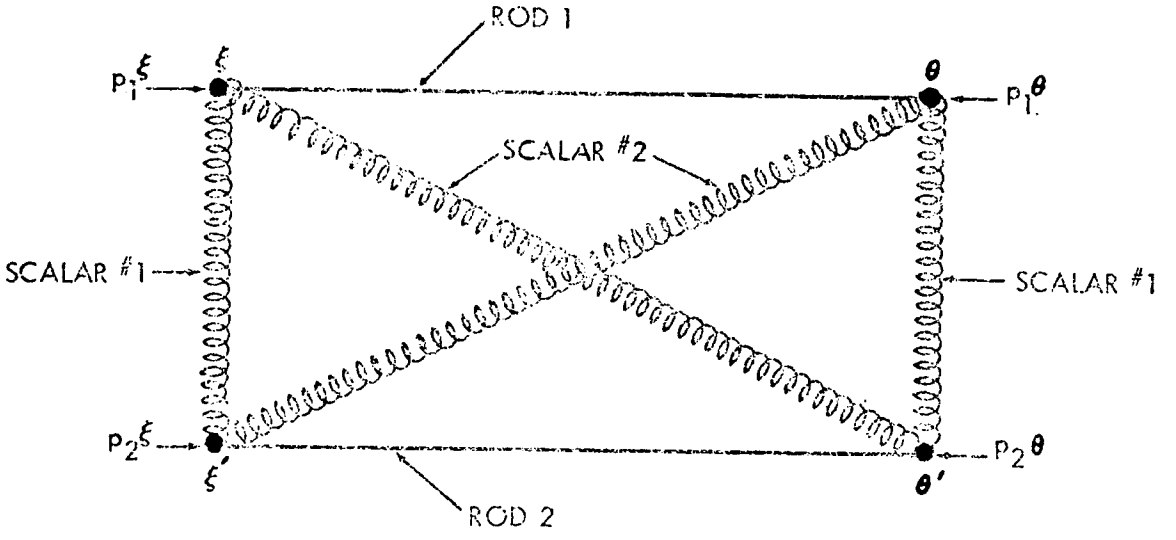
Element Connection Table for Parallel System
Connecting Grid Points 7,8,13 and 7',8',13'

Element Type	Connecting Grid Points	$\bar{t}$	Δ	$L_{\gamma\varepsilon}$	$k = -K_{coupling}$
TRIANGLE 1	7 -8 -13	2.0	0.5	2.0	
TRIANGLE 2	7'-8'-13'	2.0	0.5	4.0	
Scalar	7 -7'	2.0	0.5	1.0	$-k_{7,7'} = -1.0$
Scalar	8 -8'	2.0	0.5	1.0	$-k_{8,8'} = -2.0$
Scalar	13 -13'	2.0	0.5	1.0	$-k_{13,13'} = -1.0$
Scalar	7 -8'	2.0	0.5	1.0	$-k_{7,8'} = 1.0$
Scalar	8 -7'	2.0	0.5	1.0	$-k_{8,7'} = 1.0$
Scalar	8 -13'	2.0	0.5	1.0	$-k_{8,13'} = 1.0$
Scalar	13 -8'	2.0	0.5	1.0	$-k_{13,8'} = 1.0$
Scalar	7 -13'	2.0	0.5	1.0	$-k_{7,13'} = 0.0$
Scalar	13 -7'	2.0	0.5	1.0	$-k_{13,7'} = 0.0$

Table 4

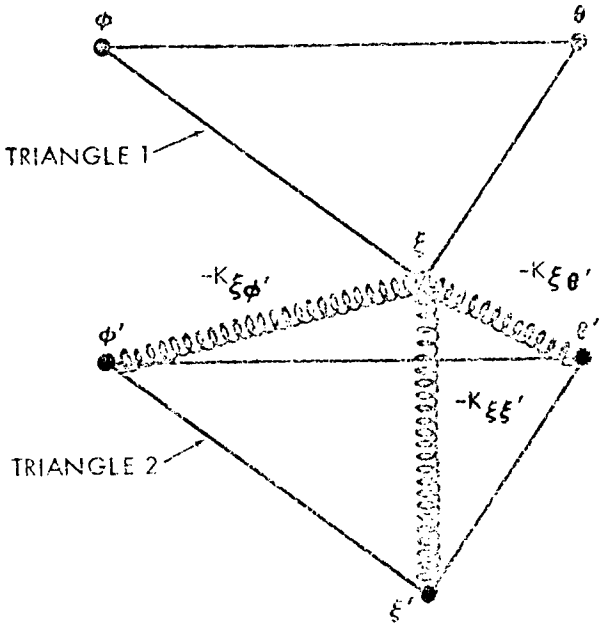
Problem 2 Results

Time	$p_1(x,y,t)$				$p_2(x,y,t)$			
	x = 2.0, y = 2.0		x = 3.0, y = 3.0		x = 2.0, y = 1.0		x = 1.0, y = 1.0	
	AN.	F.E.	AN.	F.E.	AN.	F.E.	AN.	F.E.
t=1.0	0.811	0.832	0.573	0.588	-0.811	-0.839	-0.405	-0.420
t=2.0	3.242	3.361	2.293	2.376	-3.242	-3.381	-1.621	-1.690
t=3.0	7.295	7.596	5.516	5.371	-7.295	-7.629	-3.648	-3.814
t=4.0	12.969	13.538	9.171	9.573	-12.969	-13.584	-6.485	-6.792



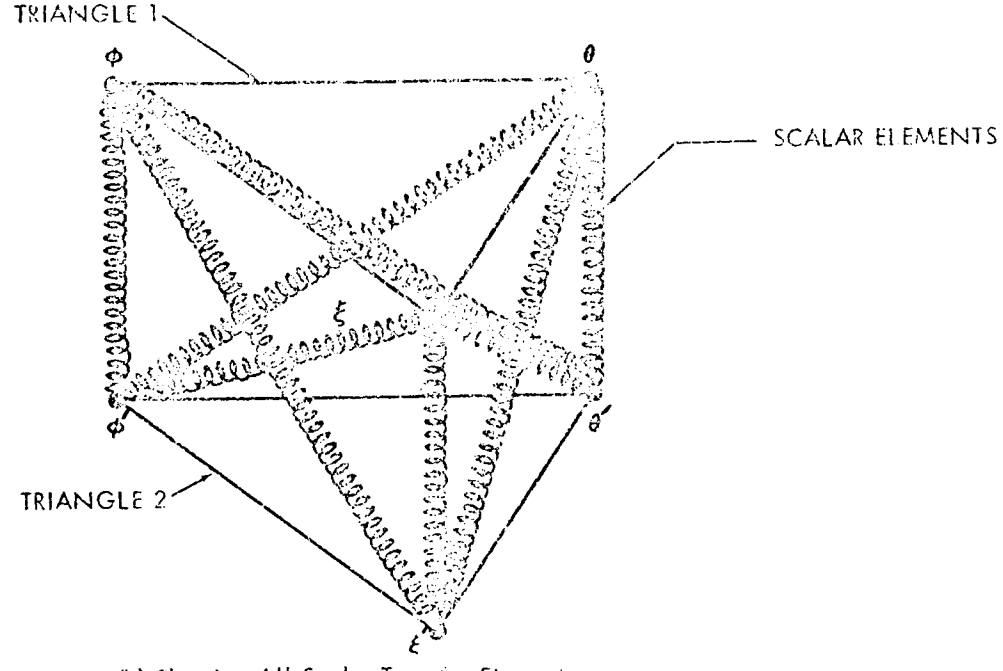
NOTE:
Geometric Coordinates of Grid Points ξ, θ
Correspond to those of ξ', θ', Respectively

Figure 1. ONE DIMENSIONAL PARALLEL ROD ELEMENT SYSTEM FOR TWO COUPLED FLOWS.



Note: Geometric Coordinates of Grid Points ξ, θ, ϕ Correspond to Those of ξ', θ', ϕ' Respectively

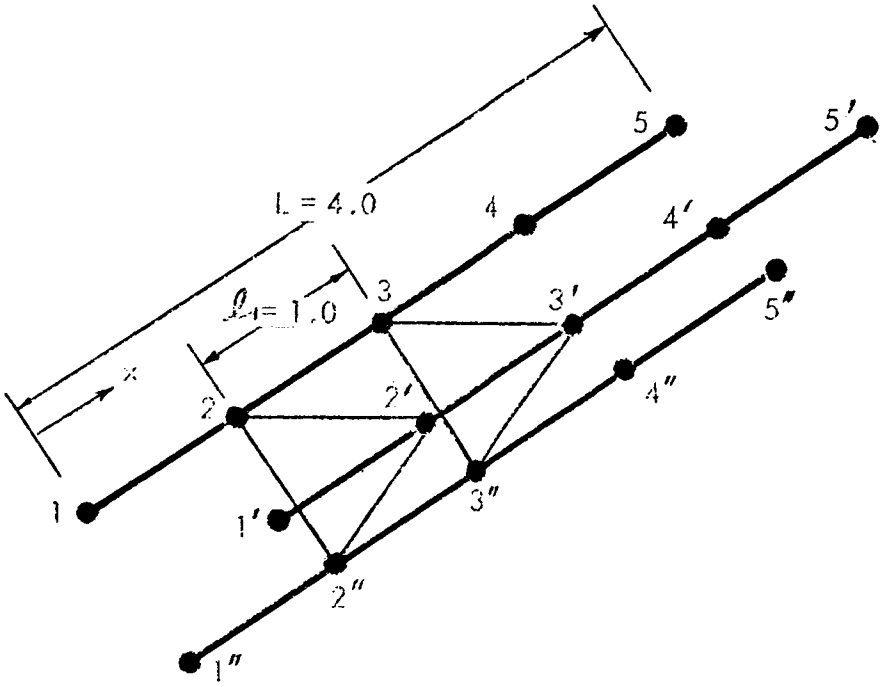
(a) Showing Typical Scalar Connections $K_{\xi\xi'}$, $K_{\xi\theta'}$, $K_{\xi\phi'}$.



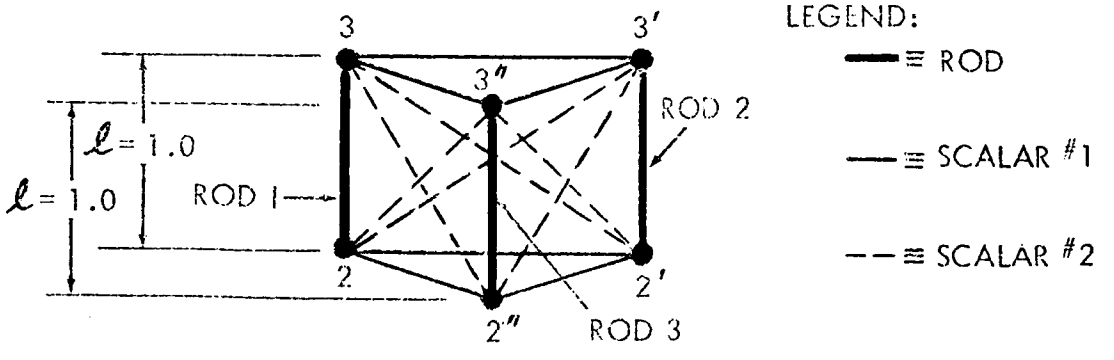
(b) Showing All Scalar Transfer Elements.

Figure 2. TWO DIMENSIONAL PARALLEL TRIANGULAR ELEMENT SYSTEM FOR TWO COUPLED FLOWS.

NOTE: Geometric Location of Grid Points 1 Through 5 Correspond to Those of 1′ Through 5′ and 1″ Through 5″, Respectively

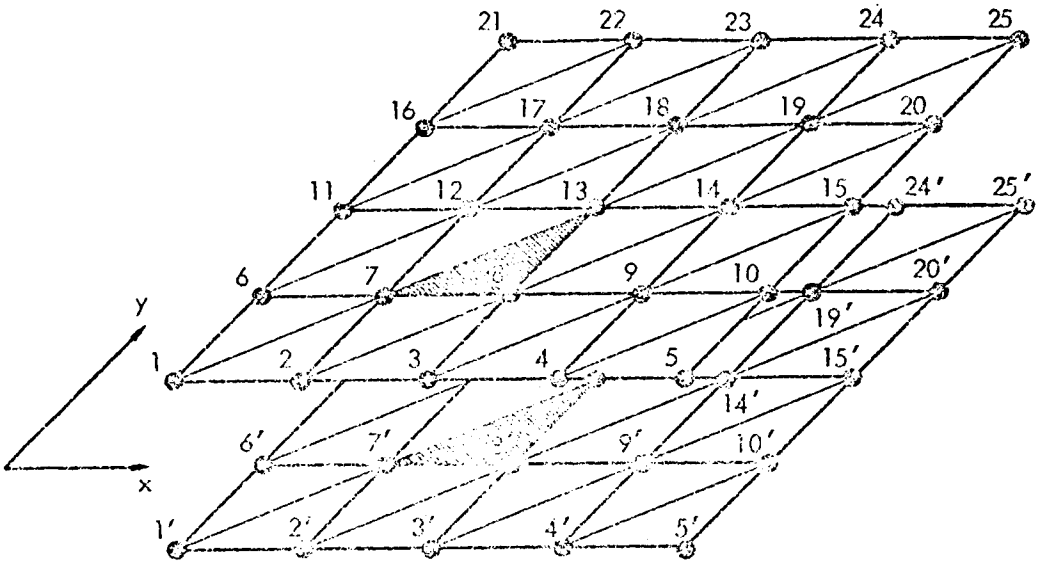


(a) Assembled Model Showing Grid Points and Parallel Rods.

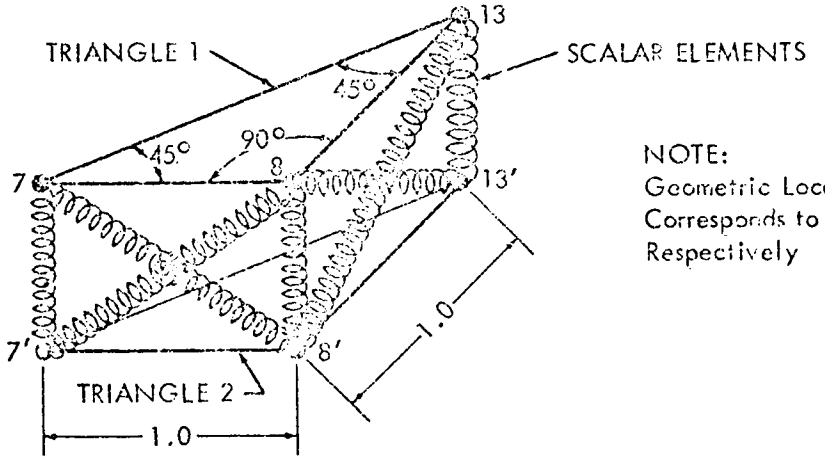


(b) Showing Typical Parallel Element System.

Figure 3. ONE DIMENSIONAL, THREE COUPLED FLOWS.



(a) Assembled Model Showing Grid Points and Parallel Triangles. (Viscous Dampers Not Shown)



NOTE:
Geometric Location of Points 1 Through 25 Corresponds to Those of 1' Through 25', Respectively

(b) Showing Typical Parallel Element System.

Figure 4. TWO DIMENSIONAL, TWO COUPLED FLOWS.